

Breakdown of universality for unequal-mass Fermi gases with infinite scattering length

D. Blume and K. M. Daily¹

¹Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, USA

(Dated: November 11, 2010)

We treat small trapped unequal-mass two-component Fermi gases at unitarity within a non-perturbative microscopic framework and investigate the system properties as functions of the mass ratio κ , and the numbers N_1 and N_2 of heavy and light fermions. While equal-mass Fermi gases with infinitely large interspecies s -wave scattering length a_s are universal, we find that unequal mass Fermi gases are, for sufficiently large κ and in the regime where Efimov physics is absent, not universal. In particular, the $(N_1, N_2) = (2, 1)$ and $(3, 1)$ systems exhibit three-body (3b) and four-body (4b) resonances at $\kappa = 12.314(2)$ and $10.4(2)$, respectively, as well as surprisingly large finite-range (FR) effects. These findings have profound implications for ongoing experimental efforts and quantum simulation proposals that utilize unequal-mass atomic Fermi gases.

PACS numbers: 03.75.Ss,05.30.Fk,34.50.-s

Dilute ultracold atomic Fermi gases have recently attracted a great deal of attention from the atomic, nuclear, particle and condensed matter communities [1]. An intriguing aspect of equal-mass two-component Fermi gases is their universality. In the regime where the interspecies s -wave scattering length a_s is much larger than the range r_0 of the underlying two-body (2b) potential, the few- and many-body behavior of dilute equal-mass Fermi gases is governed by a single microscopic parameter, namely a_s . Universality has enabled comparisons between systems with vastly different length and energy scales such as neutron matter, nuclear matter and cold atomic gases. Since the interspecies atom-atom s -wave scattering length can be tuned to essentially any value in the vicinity of a Fano-Feshbach resonance, ultracold atomic gases have emerged as an ideal model system with which to test fundamental theories such as the BCS-BEC crossover theory and to engineer and probe novel quantum phases [2].

A new degree of freedom, the mass ratio κ , comes into play when one considers unequal-mass Fermi systems such as mixtures of non-strange and strange quarks, mixtures of electrons with different effective masses [3], and dual-species cold atomic gases [4, 5]. For equal number of heavy and light fermions, the mismatch of the Fermi surfaces gives rise to novel quantum phases such as an interior gap superfluid [6]. Ultracold two-component atomic Fermi gases with unequal masses are considered to be prominent candidates with which to realize these unique phases. Most proposals along these lines assume that unequal-mass atomic Fermi systems are stable and universal. While this is true for Li-K mixtures, this Letter shows that these assumptions are, in certain regimes, violated.

We consider few-fermion systems with infinitely large interspecies s -wave scattering length a_s . The infinitely strongly interacting three-fermion system consisting of two mass m_1 fermions and one mass m_2 fermion with relative orbital angular momentum $L = 1$ and parity $\Pi = -1$ supports, within the zero-range (ZR) framework, an infinite number of 3b bound states if $\kappa \gtrsim 13.607$

$(\kappa = m_1/m_2)$ [7–9]. The properties of these states depend, as do those of bosonic $L^\Pi = 0^+$ Efimov trimers, on a_s and a so-called 3b parameter. For $8.619 \lesssim \kappa \lesssim 13.607$, 3b resonances have recently been predicted to be accessible [10]. We focus on the regime with $\kappa \lesssim 13.607$ and find: (i) The $(2, 1)$ system interacting through a purely attractive FR Gaussian interaction potential with $1/a_s = 0$ first supports, in the ZR limit, a 3b bound state in free space for $\kappa = 12.314(2)$. On resonance, the 3b bound state is, similar to a s -wave dimer, infinitely large. Away from the 3b resonance, the behavior of gas-like states of the trapped system is to a good approximation universal. (ii) Adding a light particle to the $(2, 1)$ system does not, to within our numerical resolution, lead to a new resonance. The $(3, 1)$ system, in contrast, exhibits a 4b resonance at $\kappa \approx 10.4(2)$. On the one hand, these few-body resonances open intriguing opportunities for studying weakly-bound few-body systems. On the other hand, these resonances lead to losses in experiments, thereby making the study of macroscopic unequal-mass Fermi gases more challenging. (iii) We find that unequal-mass few-fermion systems exhibit surprisingly large FR effects. This finding is relevant since a number of numerical techniques are more readily adapted to treating FR than ZR interactions. Consequently, a full theoretical understanding implies understanding FR effects. Furthermore, since realistic atom-atom interactions have a finite range, comparisons between theory and experiment have to account for FR effects.

Our calculations are performed for a trapped Fermi gas with N atoms, $N = N_1 + N_2$ (N_1 atoms with mass m_1 and N_2 atoms with mass m_2). The model Hamiltonian H reads

$$H = \sum_{j=1}^{N_1} \left(\frac{-\hbar^2}{2m_1} \nabla_{\vec{r}_j}^2 + \frac{1}{2} m_1 \omega^2 \vec{r}_j^2 \right) + \sum_{j=N_1+1}^N \left(\frac{-\hbar^2}{2m_2} \nabla_{\vec{r}_j}^2 + \frac{1}{2} m_2 \omega^2 \vec{r}_j^2 \right) + \sum_{j=1}^{N_1} \sum_{k=N_1+1}^N V_{tb}(r_{jk}), \quad (1)$$

where \vec{r}_j denotes the position vector of the j th fermion

measured with respect to the trap center and $V_{tb}(r_{jk})$ the interspecies interaction potential (here, $r_{jk} = |\vec{r}_j - \vec{r}_k|$). Intraspecies interactions are, away from an odd partial wave 2b Fano-Feshbach resonance, weak and are neglected in Eq. (1). The spherically symmetric harmonic confinement is characterized by the angular frequency ω , which determines the harmonic oscillator length a_{ho} , $a_{ho} = \sqrt{\hbar/(2\mu\omega)}$ with $\mu = m_1m_2/(m_1 + m_2)$. Throughout, we consider the infinite scattering length limit, i.e., $1/a_s = 0$. Our calculations are performed for the FR potential V_{fr} , $V_{fr}(r) = -V_0 \exp[-(r/(\sqrt{2}r_0))^2]$, with depth V_0 ($V_0 > 0$) and range r_0 ($r_0 \ll a_{ho}$). For fixed r_0 , we adjust V_0 so that the 2b system in free space is just at the verge of supporting its first s -wave bound state. For $N = 3$, our results for $V_{fr}(r)$ are compared with those for the ZR potential V_{zr} , $V_{zr}(r) = 2\pi(\hbar^2 a_s/\mu)\delta(\vec{r})\frac{\partial}{\partial r}r$.

To determine the eigenenergies of the Hamiltonian H , we separate off the center-of-mass degrees of freedom \vec{R}_{CM} and solve the Schrödinger equation in the relative coordinates. For the unitary system with ZR interactions, the relative wave function Ψ_ν separates into a hyperradial part $F_\nu(R)$ and a hyperangular part $\Phi_\nu(\vec{\Omega})$, $\Psi_\nu(R, \vec{\Omega}) = R^{-(3N-4)/2}F_\nu(R)\Phi_\nu(\vec{\Omega})$ [11]; here, R denotes the hyperradius, $\mu R^2 = \sum_{j=1}^N m_j(\vec{r}_j - \vec{R}_{CM})^2$, and $\vec{\Omega}$ collectively denotes the remaining $3N - 4$ degrees of freedom. For $N = 3$, the eigenvalues of the hyperangular Schrödinger equation can be obtained by solving a transcendental equation (see, e.g., Ref. [12]), resulting in $V_\nu(R) = \frac{\hbar^2(s_\nu^2 - 1/4)}{2\mu R^2}$. For $L^\Pi = 1^-$, the quantity s_0 —defined as the positive root of s_0^2 —decreases from 1.773 to 0 as κ increases from 1 to 13.607. For $\kappa \gtrsim 13.607$, s_0 becomes purely imaginary and Efimov physics emerges [7–9].

In a second step, the hyperradial Schrödinger equation

$$\left(\frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial R^2} + V_\nu(R) + \frac{1}{2}\mu\omega^2 R^2 \right) F_\nu(R) = E_\nu F_\nu(R) \quad (2)$$

is solved for $F_\nu(R)$ and E_ν . This differential equation has two linearly independent solutions f_ν and g_ν [13], $f_\nu(x) = A_\nu x^{s_\nu+1/2} \exp(-x^2/2) {}_1F_1(-q, s_\nu + 1, x^2)$ and $g_\nu(x) = B_\nu x^{-s_\nu+1/2} \exp(-x^2/2) {}_1F_1(-q - s_\nu, -s_\nu + 1, x^2)$, where the non-integer quantum number q is defined through $E_\nu = (2q + s_\nu + 1)\hbar\omega$ and $x = R/(\sqrt{2}a_{ho})$. We write $F_\nu(R)$ as $\cos(\pi\mu_\nu)f_\nu(R) - \sin(\pi\mu_\nu)g_\nu(R)$. Requiring that $F_\nu(R)$ vanishes at large R , the “quantum defect” μ_ν [13] is determined by the condition $\sin(\pi(\mu_\nu + q)) = 0$. Next, the allowed values of q are determined by analyzing the small R behavior. The function g_ν is only normalizable if $s_\nu < 1$ [8, 10]; this implies $\kappa > 8.619$ for the lowest hyperangular eigenvalue (i.e., $\nu = 0$). Thus, for $\kappa < 8.619$, the ZR solution is determined by the exponentially decaying piece of $f_\nu(R)$ and the quantization condition gives, in agreement with Ref. [11], $q = 0, 1, \dots$; we denote the corresponding energy by $E_{f,\nu}$ [solid lines in Fig. 1(a)]. For $\kappa > 8.619$ ($s_0 < 1$), both f_ν and g_ν can contribute [10] and the eigenenergy depends on the boundary condition

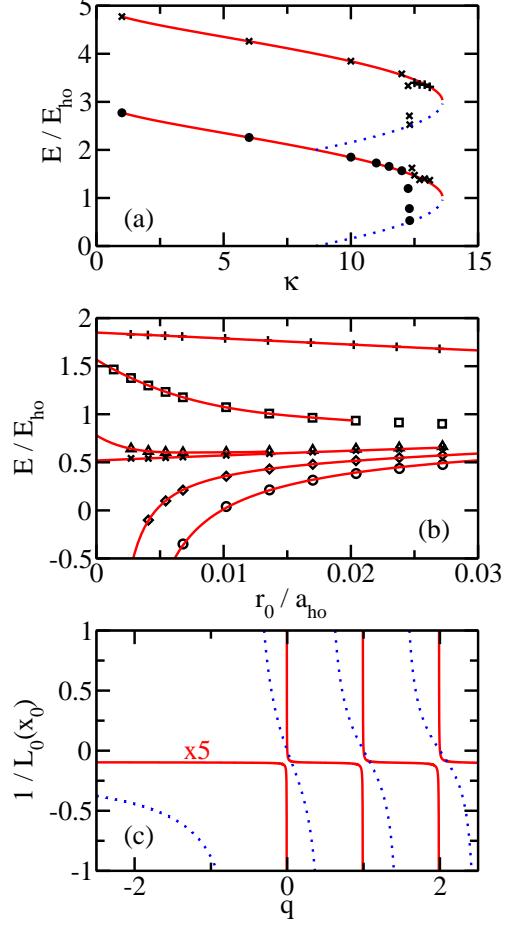


FIG. 1: (Color online) (2,1) system with $L^\Pi = 1^-$ at unitarity. (a) Circles, crosses and pluses show the SV energies, extrapolated to the ZR limit, for the three energetically lowest-lying states as a function of κ . Solid and dotted lines show $E_{f,0}$ ($q = 0$ and 1) and $E_{g,0}$ ($q = -s_0$ and $-s_0 + 1$), respectively. (b) Pluses, squares, triangles, crosses, diamonds and circles show the lowest SV energy for $\kappa = 10, 12, 12.3, 12.314, 12.4$ and 12.5 , respectively, as a function of r_0 . Solid lines show fits to the SV energies. (c) Dotted and solid lines show $1/L_0(x_0)$ for $x_0 = 0.001$ as a function of q for $s_0 = 1/2$ ($\kappa \approx 12.3131$) and $s_0 = 11/20$ ($\kappa \approx 12.0449$), respectively. The data for $s_0 = 11/20$ are scaled by a factor of 5 for enhanced readability. In the ZR limit, the resonance condition implies $q = -1/2, 1/2, \dots$ for $s_0 = 1/2$ and $q = -11/20, 9/20, \dots$ for $s_0 = 11/20$ (see text for details).

(BC) at small R . Just as in the case of Efimov trimers, this BC is determined by the true atom-atom interactions and cannot be derived within the ZR framework. Parameterizing the BC by the log derivative $L_\nu(x_0)$, where $L_\nu(x_0) = [F'_\nu(x)/F_\nu(x)]_{x=x_0}$, the allowed q values can be obtained as a function of $L_\nu(x_0)$. Figure 1(c) shows $[L_0(x_0)]^{-1}$ as a function of q for $s_0 = 1/2$ and $11/20$. If only g_ν contributes, we find, in agreement with note [43] of Ref. [11], $q = -s_\nu, -s_\nu + 1, \dots$ in the ZR limit. The corresponding energies $E_{g,0}$ are shown by dotted lines in

Fig. 1(a). In the following, we determine the 3b spectrum for the FR potential $V_{\text{fr}}(r)$ by the stochastic variational (SV) method, which makes no assumption about the small R behavior of $F_\nu(R)$, and interpret it using Fig. 1(c).

The SV approach [14] expands the relative wave function in terms of a basis set. The proper antisymmetrization of the basis functions, which are optimized semi-stochastically, is enforced explicitly through the application of permutation operators. The resulting eigenenergies $E(N_1, N_2)$ of the relative Hamiltonian provide an upper bound to the exact eigenenergies. The functional form of the basis functions used depends on the state of interest [14]. For natural parity states, we use a spherical harmonic that depends on a generalized coordinate and multiply it by a product of Gaussians in the relative distance coordinates. In this case, the basis functions have definite parity and angular momentum. To describe unnatural parity states, we employ so-called geminal type basis functions that have neither good parity nor good angular momentum and select the state of interest from the entirety of states.

Symbols in Fig. 1(b) show selected SV energies for the $(2, 1)$ system with $L^\Pi = 1^-$ at unitarity as a function of r_0 . To extrapolate to the $r_0 \rightarrow 0$ limit, we perform 4-5 parameter fits to the SV energies [solid lines in Fig. 1(b)]. The resulting extrapolated ZR energies are shown by symbols in Fig. 1(a). The key characteristics of Figs. 1(a) and 1(b) can be summarized as follows: (i) The dependence of the 3b energy on r_0 increases as κ increases from 1 to about 12. For $\kappa = 12$, e.g., the difference between the extrapolated ZR energy and the energy for $r_0 = 0.01a_{\text{ho}}$ is about 30%. For $\kappa = 12.314$, the energy depends comparatively weakly on r_0 . (ii) For $\kappa = 12.4$ and 12.5, the ground state energy is negative for sufficiently small r_0 and diverges as r_0^{-2} with decreasing r_0 . (iii) For $\kappa \neq 12.314$ and $\kappa = 12.314$, the extrapolated ZR energies [symbols in Fig. 1(a)] agree to a very good approximation with $E_{f,0}$ and $E_{g,0}$, respectively. We interpret the dropping of the energy around $\kappa \approx 12.3$ ($s_0 \approx 1/2$) as a 3b resonance. The resonance position is found to be $\kappa = 12.314(2)$.

Although the occurrence of the 3b resonance depends on the underlying 2b potential, we now argue that a 3b resonance occurs most likely if $s_0 \approx 1/2$. The hyperradial wave function of the 3b system with FR interactions is for $R \gtrsim r_0$ given by F_ν . Figure 1(c) shows the dependence of the allowed quantum numbers q on the value of $1/L_0(x_0)$ for $x_0 = 0.001$. For $s_0 \neq 1/2$ [the solid line in Fig. 1(c)] shows an example for $s_0 = 11/20$, nearly all values of the logderivative result in $q \approx 0, 1, \dots$, implying that the realization of a 3b resonance for $s_0 \neq 1/2$ requires careful fine-tuning (as x_0 decreases, the “corners” of the solid line near integer q values become even sharper). If realized, such a resonance is narrow, with the size of the zero-energy trimer set—as in the case of non-universal p -wave dimers—by the effective angular momentum barrier. Physically, an unnaturally large contribution of g_ν

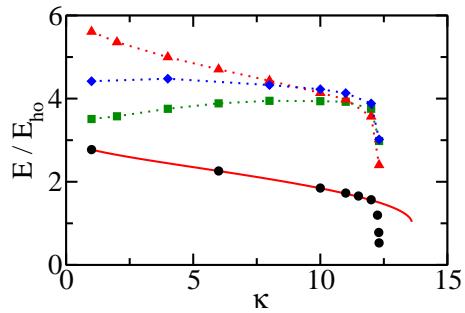


FIG. 2: (Color online) Squares, triangles and diamonds show the extrapolated ZR ground state energies of the $(2, 2)$ system with $L^\Pi = 0^+, 1^-$ and 2^+ , respectively. The extrapolation to the ZR limit is based on 3-5 parameter fits to the SV energies for $r_0 \approx 0.005a_{\text{ho}}$ to $0.02a_{\text{ho}}$. Circles and a solid line show the energies of the $(2, 1)$ system with $L^\Pi = 1^-$ [see Fig. 1(a)].

is, for $s_0 > 1/2$, “suppressed” by the effective repulsive angular momentum barrier in the hyperradial coordinate. For $s_0 = 1/2$ [dotted line in Fig. 1(c)], in contrast, the resonance is broad and on resonance the size of the zero-energy trimer in free space is, much like that of s -wave dimers at unitarity, infinite. Our analysis of the structural properties such as the hyperradial density for FR systems confirms this conclusion. Since the effective angular momentum barrier vanishes for $s_0 = 1/2$, g_ν is no longer naturally suppressed and the existence of a 3b resonane is more probable. While our analysis shows a 3b resonance occurs more likely if $s_0 \approx 1/2$, the ZR model cannot predict whether or not such a resonance does indeed occur. Based on the FR results presented in Figs. 1(a) and (b), we speculate that other classes of interaction potentials likely also support a 3b resonance near $s_0 \approx 1/2$.

We now investigate the $(2, 2)$ and $(3, 1)$ systems, i.e., we add respectively a light and a heavy atom to the $(2, 1)$ system. Symbols in Fig. 2(a) show the extrapolated ZR energies for the lowest natural parity states of the $(2, 2)$ system with $L = 0 - 2$. The FR effects are comparable to those of the $(2, 1)$ system discussed in the context of Fig. 1 [15]. The uncertainty of the SV energies is less than 1% and the uncertainty of the extrapolated ZR energies is primarily due to the fact that our SV calculations for the $(2, 2)$ systems are limited to $r_0 \gtrsim 0.005a_{\text{ho}}$. For all three L considered, the $(2, 2)$ energies lie above the $(2, 1)$ energies and show a notable drop at $\kappa \approx 12.3$, which we attribute to the presence of the 3b resonance. Our calculations show no evidence for a $(2, 2)$ resonance. We also considered unnatural states of the $(2, 2)$ system and find that the lowest unnatural parity state lies above the lowest natural parity state.

We now show that the $(3, 1)$ system exhibits a 4b resonance at a κ value that differs from that at which the 3b resonance occurs. The energetically lowest lying state of the $(3, 1)$ system has $L = 1$ and unnatural parity. Our extrapolated ZR energies are $5.1\hbar\omega$, $4.9\hbar\omega$, $4.5\hbar\omega$ and

$3.9\hbar\omega$ for $\kappa = 1, 2, 4$ and 8 , respectively. While our calculations for larger κ do not allow for a reliable extrapolation to the ZR limit, they do allow for a reliable determination of the $(3, 1)$ resonance position. To locate the resonance position, we monitor whether the SV energies decrease or increase with decreasing r_0 . For $\kappa = 10$, e.g., we find that the energy increases with decreasing r_0 . For $\kappa = 10.6$, in contrast, we find negative energies for $r_0 \lesssim 0.02a_{ho}$. Performing additional calculations for $\kappa = 10.3, 10.4$ and 10.5 , we find that the $(3, 1)$ resonance is located at $\kappa = 10.4(2)$. As in the $(2, 1)$ case, the exact position of the $(3, 1)$ resonance depends on the details of the underlying 2b interactions. In particular, the analysis of the small R BC of the hyperradial wave function of the $(3, 1)$ system parallels that of the $(2, 1)$ system. This implies that the smallest mass ratio at which a $(3, 1)$ resonance can occur depends on the solution to the hyperangular Schrödinger equation, i.e., the s_0 of the $(3, 1)$ system needs to be smaller than 1 . It appears likely that the $(4, 1), (5, 1)$, etc. systems exhibit resonances at successively smaller κ .

In summary, we considered unequal-mass two-component Fermi gases interacting through FR potentials with infinite interspecies s -wave scattering length a_s and found 3b and 4b resonances in regimes where Efimov physics is absent. These resonances are non-universal in the sense that their exact position and properties depend

on, besides a_s , at least one additional parameter. We argued that 3b resonances occur most likely if $\kappa \approx 12.3$ ($s_0 \approx 1/2$) and that 4b systems likely exhibit, assuming a 3b resonance exists near $s_0 \approx 1/2$, a 4b resonance near $\kappa \approx 10.4$. While we adjusted s_0 by varying κ , experimentalists could tune the N -body s_0 by utilizing an intraspecies Fano-Feshbach resonance [10]. Importantly, our results for the $(N_1, 1)$ systems apply not only to Fermi-Fermi mixtures but also to Fermi-Bose mixtures, making the ${}^7\text{Li}-{}^{87}\text{Sr}$ system ($\kappa \approx 12.4$)—thanks to the existence of optical Sr-Sr Fano-Feshbach resonances [16]—a promising candidate for experimental studies. We note that the 3b resonance discussed here differs from the resonances discussed in Ref. [12] for positive a_s . The breakdown of universality and the instability of unequal-mass atomic Fermi gases discussed in this work also provides opportunities: Our theoretical study paves the way for exciting investigations of novel few- and many-body systems with simultaneous 2b and 3b or 2b and 4b resonances, either in a dipole trap or an optical lattice set-up.

After completion of our manuscript, we received a related, independent manuscript by S. Gandolfi and J. Carlson [17]; see also talk by J. Carlson on 03/11/10, http://www.int.washington.edu/talks/WorkShops/int_10_46W/.

Support by the NSF (grant PHY-0855332) and ARO as well as fruitful discussions with J. Carlson, S. Tan and J. von Stecher are gratefully acknowledged.

-
- [1] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).
- [2] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008). W. Ketterle and M. W. Zwierlein, Rivista del Nuovo Cimento **31**, 247 (2008).
- [3] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. **3**, 552 (1959).
- [4] For Li-K, see M. Taglieber *et al.*, Phys. Rev. Lett. **100**, 010401 (2008). A number of groups are currently pursuing the trapping and cooling of mixtures containing combinations of Li, K, Sr and Yb.
- [5] S.-T. Wu, C.-H. Pao, and S.-K. Yip, Phys. Rev. B **74**, 224504 (2006). C.-H. Pao, S.-T. Wu, and S.-K. Yip, Phys. Rev. A **76**, 053621 (2007). M. M. Parish, F. M. Marchetti, A. Lamacraft, and B. D. Simons, Phys. Rev. Lett. **98**, 160402 (2007). J. von Stecher, C. H. Greene, and D. Blume, Phys. Rev. A **76**, 053613 (2007). M. A. Baranov, C. Lobo, and G. V. Shlyapnikov, *ibid.* **78**, 033620 (2008). D. Blume, *ibid.* **78**, 013613 (2008). G. Orso, L. P. Pitaevskii, and S. Stringari, *ibid.* **77**, 033611 (2008). I. Bauschert, A. Recati, and S. Stringari, *ibid.* **79**, 043622 (2009). A. Gezerlis, S. Gandolfi, K. E. Schmidt, and J. Carlson, Phys. Rev. Lett. **103**, 060403 (2009). R. B. Diener and M. Randeria, Phys. Rev. A **81**, 033608 (2010).
- [6] W. V. Liu and F. Wilczek, Phys. Rev. Lett. **90**, 047002 (2003).
- [7] V. N. Efimov, Yad. Fiz. **12**, 1080 (1970) [Sov. J. Nucl. Phys. **12**, 589 (1971)]. V. Efimov, Nucl. Phys. A **210**, 157 (1973).
- [8] D. S. Petrov, Phys. Rev. A **67**, 010703(R) (2003).
- [9] J. P. D’Incao and B. D. Esry, Phys. Rev. A **73**, 030702(R) (2006); *ibid* **73**, 030703(R) (2006).
- [10] Y. Nishida, D. T. Son, and S. Tan, Phys. Rev. Lett. **100**, 090405 (2008).
- [11] F. Werner and Y. Castin, Phys. Rev. A **74**, 053604 (2006).
- [12] O. I. Kartavtsev and A. V. Malykh, J. Phys. B **40**, 1429 (2007).
- [13] B. Borca, D. Blume, and C. H. Greene, New J. Phys. **5**, 111 (2003). We generalize the quantum defect theory approach of this reference from $s_\nu = 1/2$ to arbitrary s_ν .
- [14] Y. Suzuki and K. Varga, *Stochastic Variational Approach to Quantum Mechanical Few-Body Problems* (Springer Verlag, Berlin, 1998). H. H. B. Sørensen, D. V. Fedorov and A. S. Jensen, in *Nuclei and Mesoscopic Physics*, AIP Conf. Proc. No. 777, edited by V. Zelevinsky (AIP, Melville, NY, 2005), p. 12. J. von Stecher and C. H. Greene, Phys. Rev. Lett. **99**, 090402 (2007). K. M. Daily and D. Blume, Phys. Rev. A **81**, 053615 (2010).
- [15] The FR effects were underestimated in J. von Stecher, C. H. Greene and D. Blume, Phys. Rev. A **77**, 043619 (2008).
- [16] R. Ciurylo, E. Tiesinga, and P. S. Julienne, Phys. Rev. A **71**, 030701(R) (2005). K. Enomoto, K. Kasa, M. Kitagawa, and Y. Takahashi, Phys. Rev. Lett. **101**, 203201 (2008).
- [17] S. Gandolfi and J. Carlson, arXiv:1006.5186.